Variability of Profile Shapes for O_3 and NO_2 and Comparison to Simulated Profiles during the DISCOVER-AQ Project

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Investigation Overview

Deriving Information on Surface Conditions from Column and VERtically Resolved Observations Relevant to Air Quality

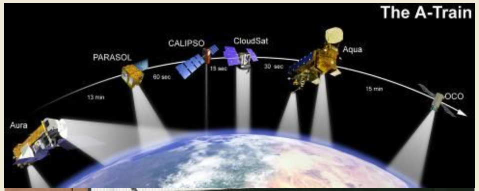
A NASA Earth Venture campaign intended to improve the interpretation of satellite observations to diagnose near-surface conditions relating to air quality

Objectives:

1. Relate column observations to surface conditions for aerosols and key trace gases O_3, NO_2, and CH_2O

2. Characterize differences in diurnal variation of surface and column observations for key trace gases and aerosols

3. Examine horizontal scales of variability affecting satellites and model calculations



Deployments and key collaborators

Maryland, July 2011 (EPA, MDE, UMd, and Howard U.)
SJV, California, January/February 2013 (EPA and CARB)
Texas, September 2013 (EPA, TCEQ, and U. of Houston)
Colorado, Summer 2014

Deployment Strategy

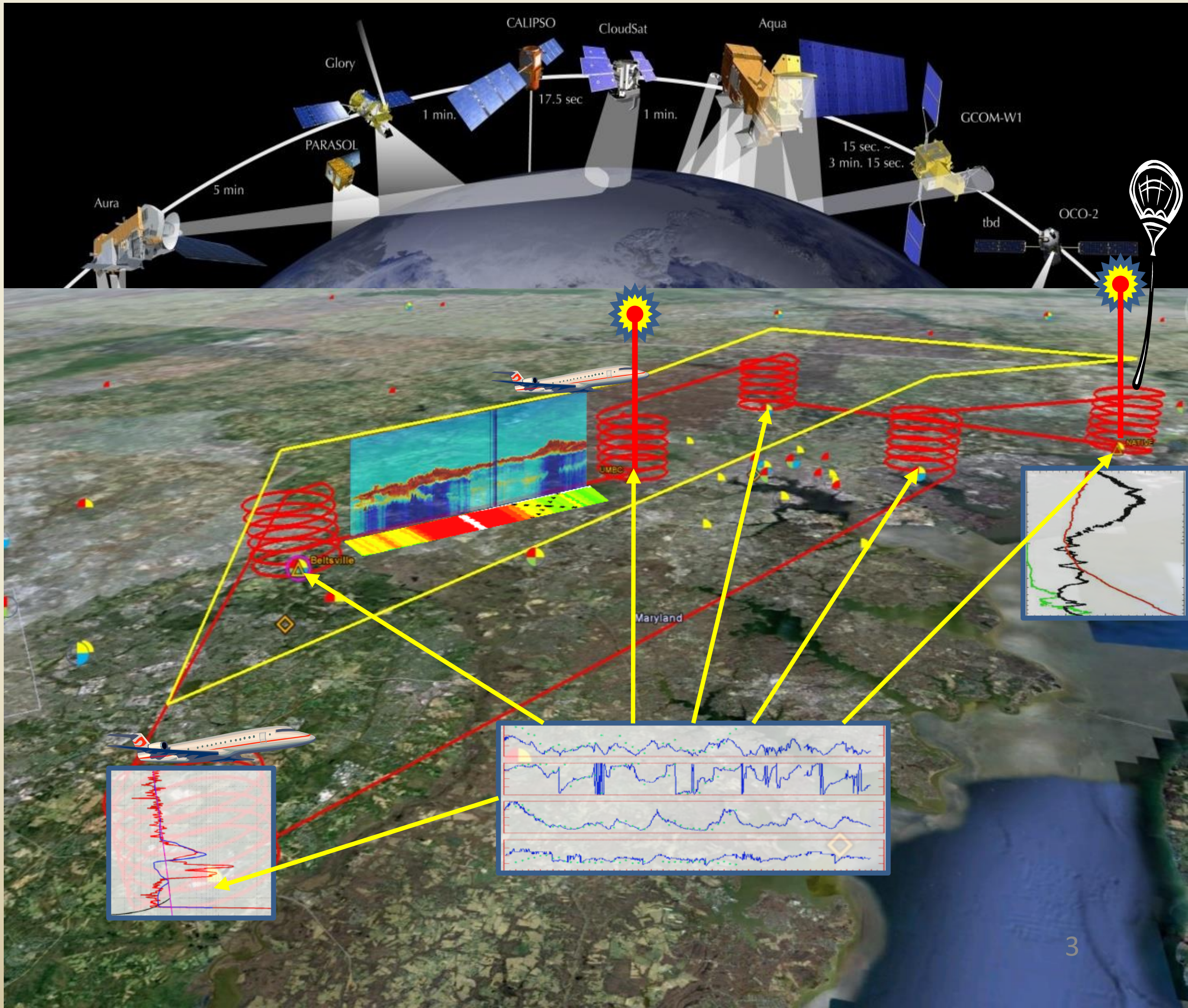
Systematic and concurrent observation of column-integrated, surface, and vertically-resolved distributions of aerosols and trace gases relevant to air quality as they evolve throughout the day.

Three major observational components:

<u>NASA UC-12 (Remote sensing)</u>
Continuous mapping of aerosols with HSRL and trace gas columns with ACAM

<u>NASA P-3B (in situ meas.)</u>
In situ profiling of aerosols and trace gases over surface measurement sites

<u>Ground sites</u>
In situ trace gases and aerosols
Remote sensing of trace gas and aerosol columns (Pandora)
Ozonesondes
Aerosol lidar observations



Motivation

- Understanding variability of *in situ* profile shapes is useful for understanding how column data and surface data are related
  - Profile shape determines which altitude layers contribute most to the column
  - Ultimately, how well do satellite observations represent surface air quality?

- Also useful in the assessment of air quality models and the assumed profile shapes used in satellite retrievals

- Objective of this study is to characterize the variability of the *in situ* O_3 and NO_2 P-3B profiles
  - Do classes of profile shapes emerge for each campaign?
  - How well do regional and global air quality model simulated profiles compare to the observations?

Hierarchical Cluster Analysis

- Followed the approach of Hains et al. (2008)
  - Agglomerative hierarchical cluster analysis
  - P-3B O_3 or NO_2 profiles only
  - Applied to each of the 4 campaigns

- Cluster analysis seeks to group together similar objects (objects can be individual differences between profile pairs, or even clusters of profile differences)

- Initially treats each object (individual differences) as its own cluster and continues to cluster until all objects (individual differences/clusters of differences) are grouped into one large cluster

Hains, J. C., Taubman, B. F., Thompson, A. M., Stehr, J. W., Marufu, L. T., Doddridge, B. G., Dickerson, R. R. (2008), Origins of chemical pollution derived from Mid-Atlantic aircraft profiles using a clustering technique, *Atmos. Env.*, 42, 1727-1741

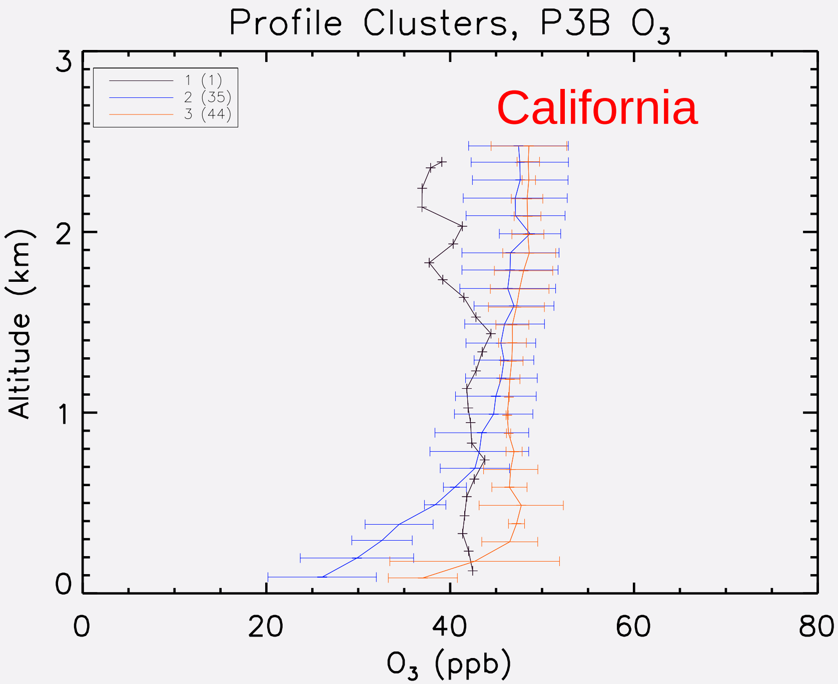
Hierarchical Cluster Analysis

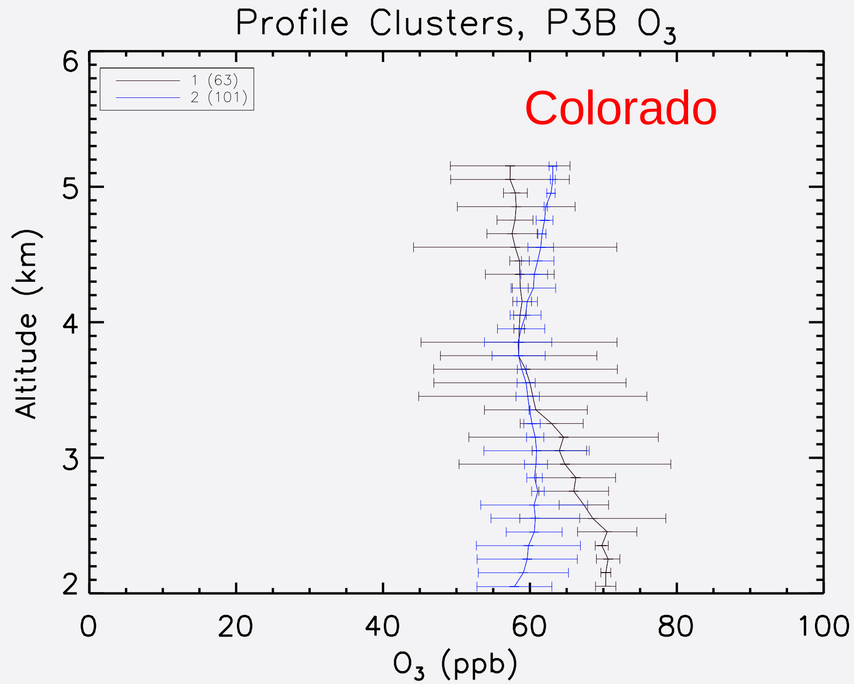
- Optimal number of meaningful clusters determined by combination of manual inspection of dendrogram, rules of thumb, and a technique based on total root mean square deviation (TRMSD)

- Median profile cluster significance criterion:
  - 5 consecutive altitude layers in which the error bars did not overlap with those of any other median profile

Hains, J. C., Taubman, B. F., Thompson, A. M., Stehr, J. W., Marufu, L. T., Doddridge, B. G., Dickerson, R. R. (2008), Origins of chemical pollution derived from Mid-Atlantic aircraft profiles using a clustering technique, *Atmos. Env.*, 42, 1727-1741

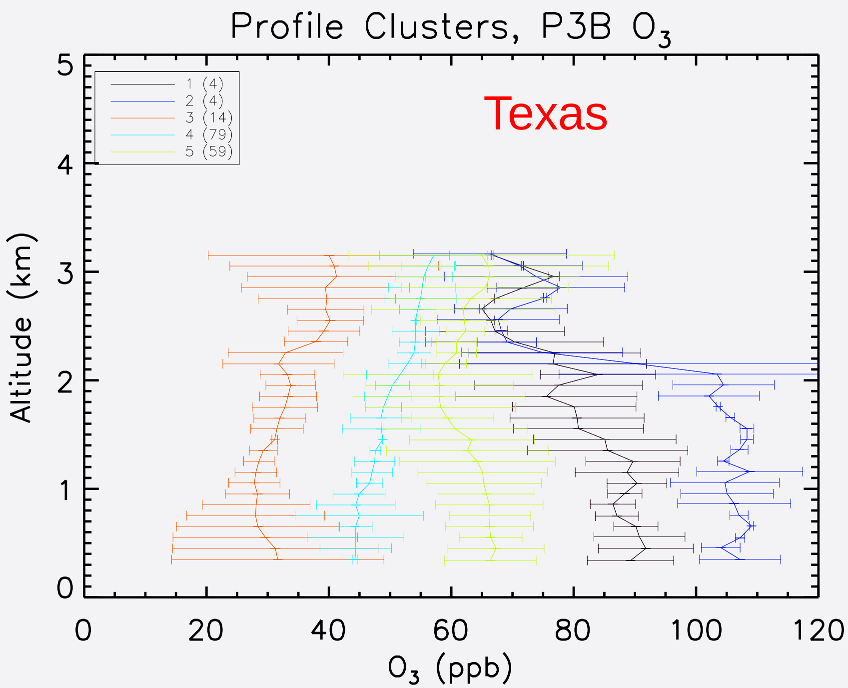
P-3B O_3 Cluster Median Profiles

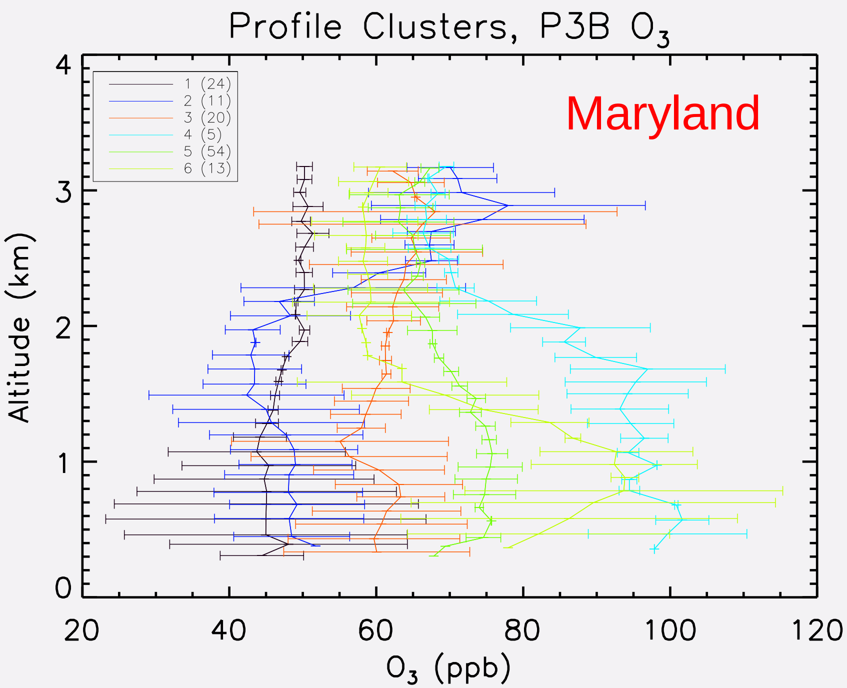




- Few clusters obtained for the California and Colorado campaigns
  - Complex terrain may lead to greater horizontal mixing within study region
  - CA campaign occurred during cold season
  - However, all clusters significant within planetary boundary layer (PBL)

P-3B O_3 Cluster Median Profiles



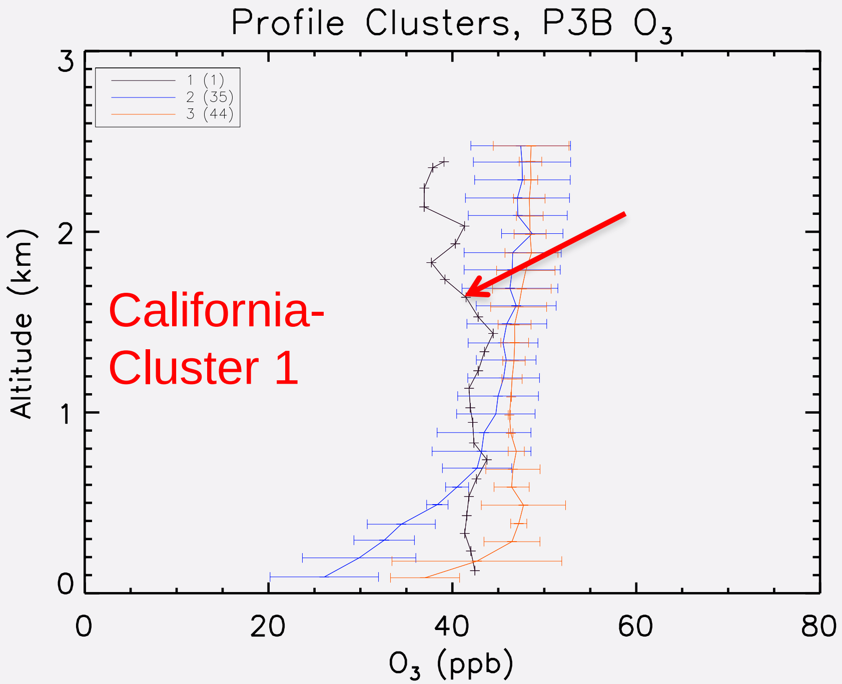


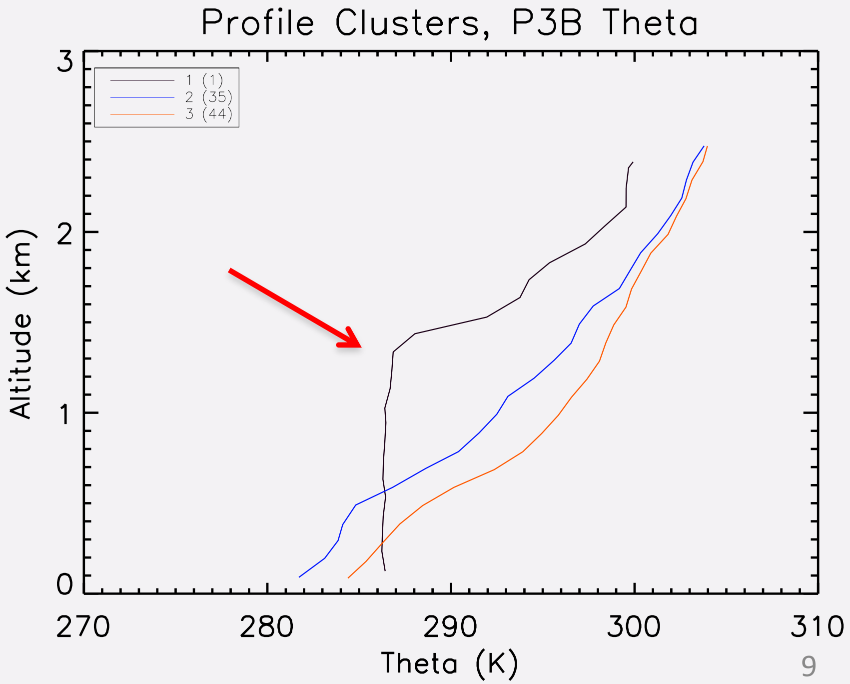
- Texas demonstrated the greatest number of significant clusters
  - Greatest range of mixing ratio values also

- Maryland's behavior unlike the other 3 campaigns
  - Appears to produce the most clusters, but only Cluster 4 is distinct within mid-upper PBL

Influence of Vertical Mixing

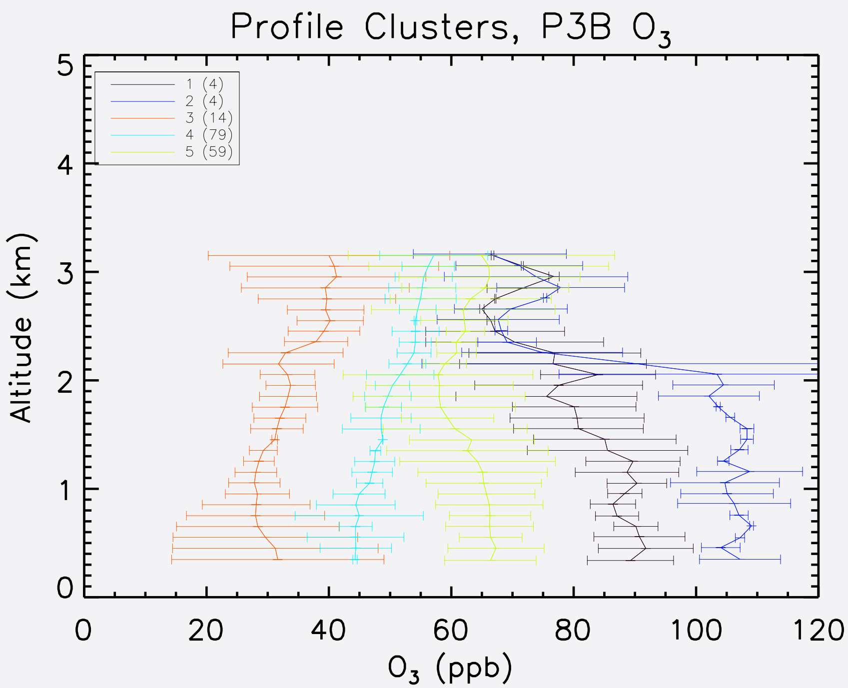
- Potential temperature (theta) profile indicates stability and degree of vertical mixing within PBL, FT
- Generally, where the theta profile is well mixed within the PBL, the O_3 profile is also relatively well mixed and vice versa

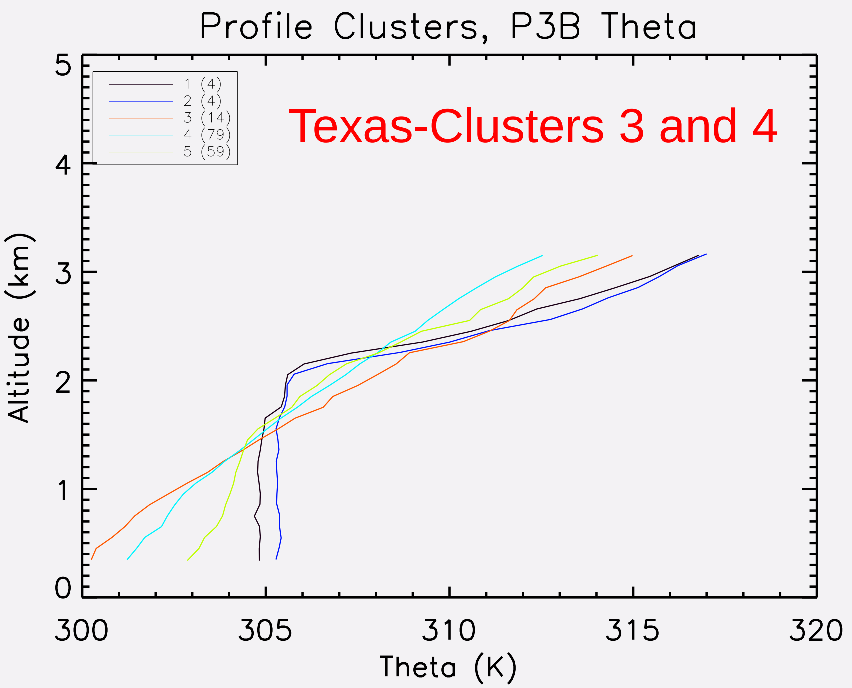




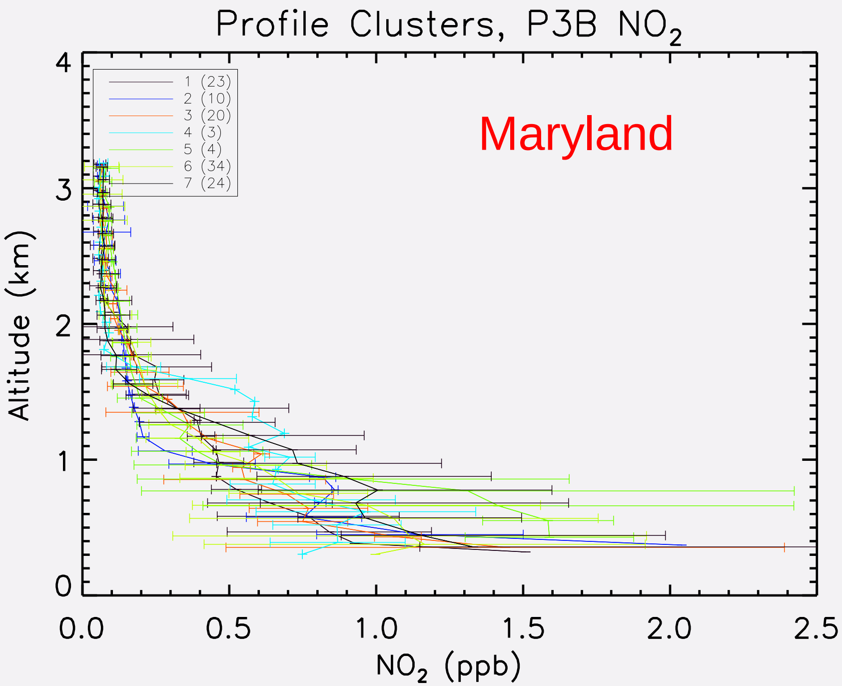
Influence of Vertical Mixing

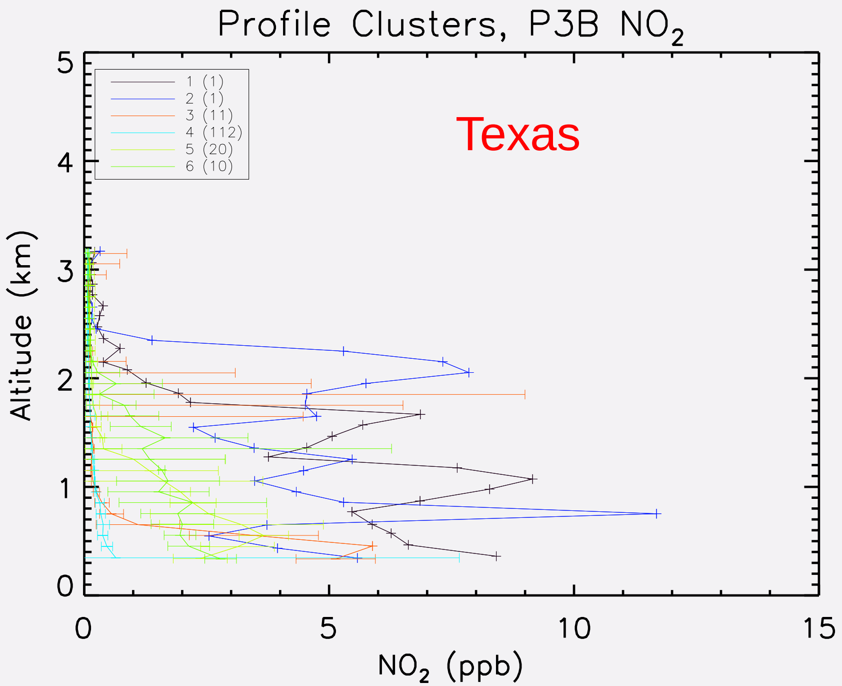
- However, influence of vertical mixing somewhat weaker for MD, TX campaigns than for CA, CO campaigns





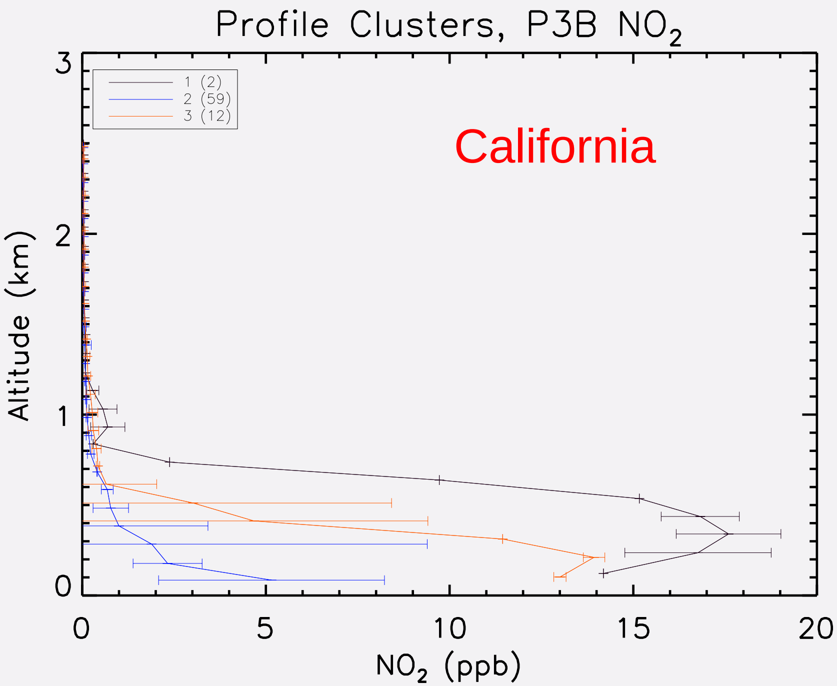
P-3B NO_2 Cluster Median Profiles

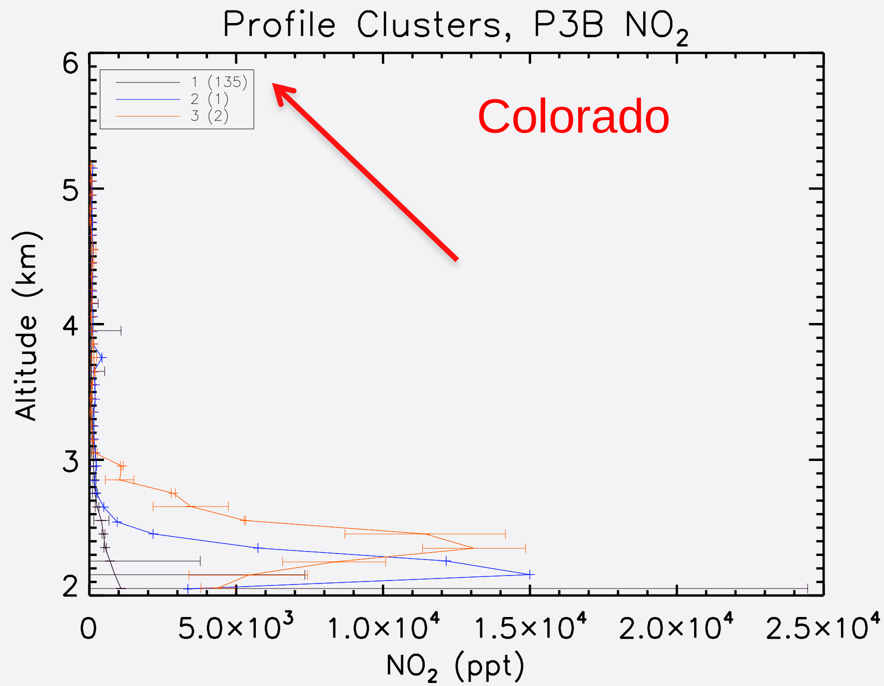




- Maryland again produced greatest number of clusters though none are significant
- Clusters 1 and 2 (with 1 profile apiece) only are significant for the Texas campaign
- NO_2 profiles thus displayed relatively uniform behavior

P-3B NO_2 Cluster Median Profiles





- All 3 clusters are significant for these campaigns, but……
- Only California hints at some NO_2 profile variability
- NO_2 again fairly uniform behavior
- Larger mixing ratios encountered during CA, CO than for MD, TX

Influences on NO_2

- No clear meteorological influences emerged at the spiral sampling times (potential temperature, lapse rate, winds, etc.)

- Mixing ratio ranges, number of significant clusters suggest O_3 production plays a role in regulating the variability of the NO_2 profile behavior
  - More profile shape variability under conditions of inhibited O_3 formation and vice versa

Model Simulations

- Different model simulations available for different campaigns
- Community Multiscale Air Quality (CMAQ) model:

  - Simulations available for the Maryland and Texas campaigns courtesy of Chris Loughner (NASA GSFC)

  - NOAA ARL CMAQ forecasts available for the California, Colorado campaigns

Loughner et al. CMAQ Simulations

	Maryland	Texas
Time Period	May 25 through July 31, 2011	Aug. 18 through Sept. 31, 2013
Chemical mechanism	CB05	CB05
Aerosols	AE5	AE5
Domain	12 km horizontal resolution over eastern U. S.	4 km horizontal resolution over eastern TX
Inputs	WRF meteorology; MOZART CTM	WRF meteorology; MOZART CTM
Vertical Diffusion	ACM2	ACM2
Land Surface Model	Pleim-Xiu	Pleim-Xiu
LNOx	Yes	Yes

NOAA CMAQ Forecasts

	California	Colorado
Time Period	January-February 2013	July-August 2014
Chemical mechanism	CB05	CB05
Aerosols	aero4	Aero4
Domain	12 km horizontal resolution over continental U. S.	4 km horizontal resolution over Colorado
Inputs	WRF meteorology	WRF meteorology
Vertical Diffusion	MYJ	MYJ
Land Surface Model	NOAH LSM	NOAH LSM

O_3 and NO_2 Shape Factors

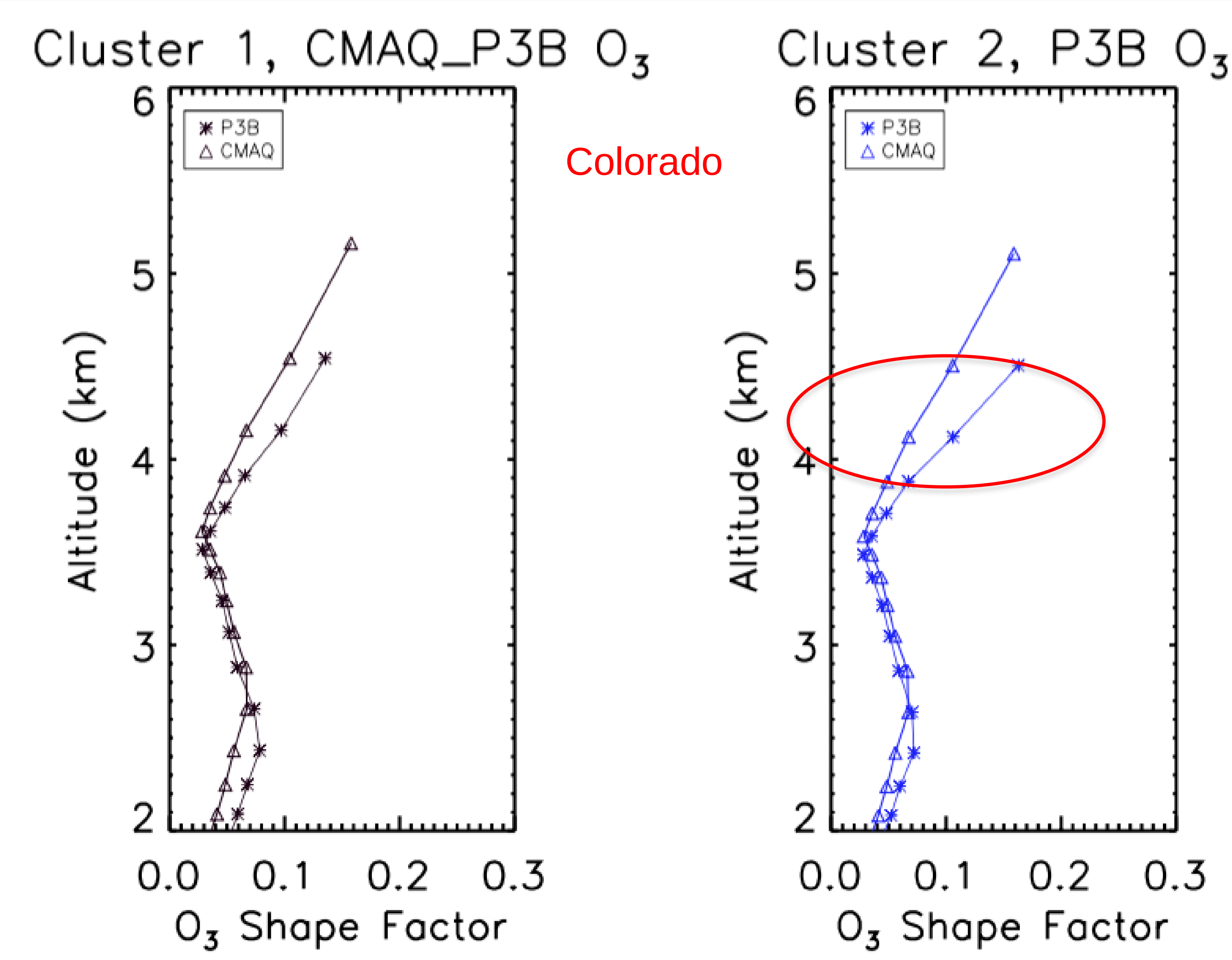
- Median shape factor for O_3 and NO_2 also computed for each cluster

- Shape factor defined as ratio of partial column within a model vertical layer to the tropospheric column
    - $S(z) = \Omega_z/\Omega_{trop}$

- Computed for P-3B profiles
    - Partial column computed for CMAQ layer
    - Ratio to P-3B partial tropospheric column then computed

- Also computed for CMAQ profiles
    - Also used partial column over P-3B spiral depths for comparison!!

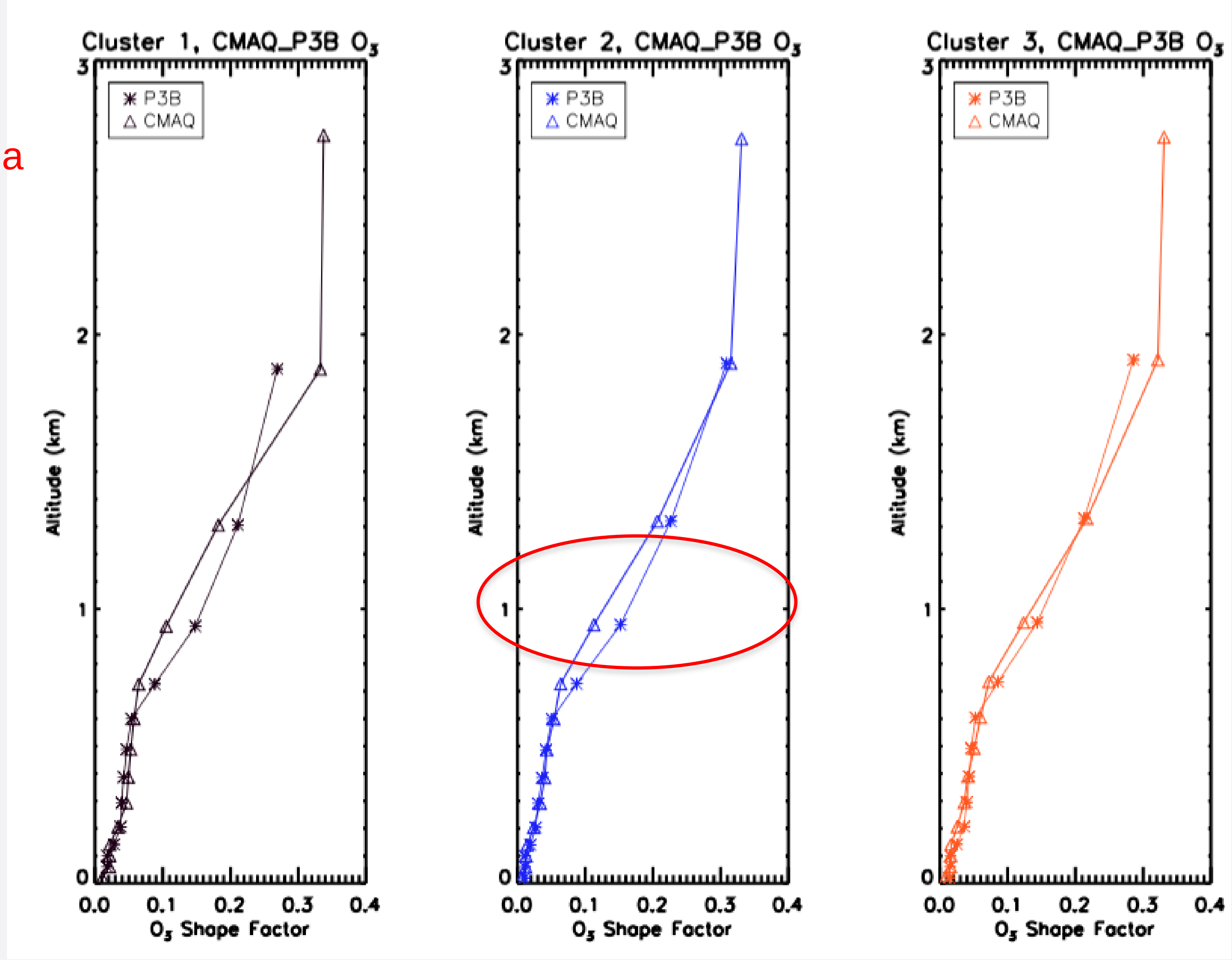
P3B/CMAQ O_3 Shape Factors



Colorado

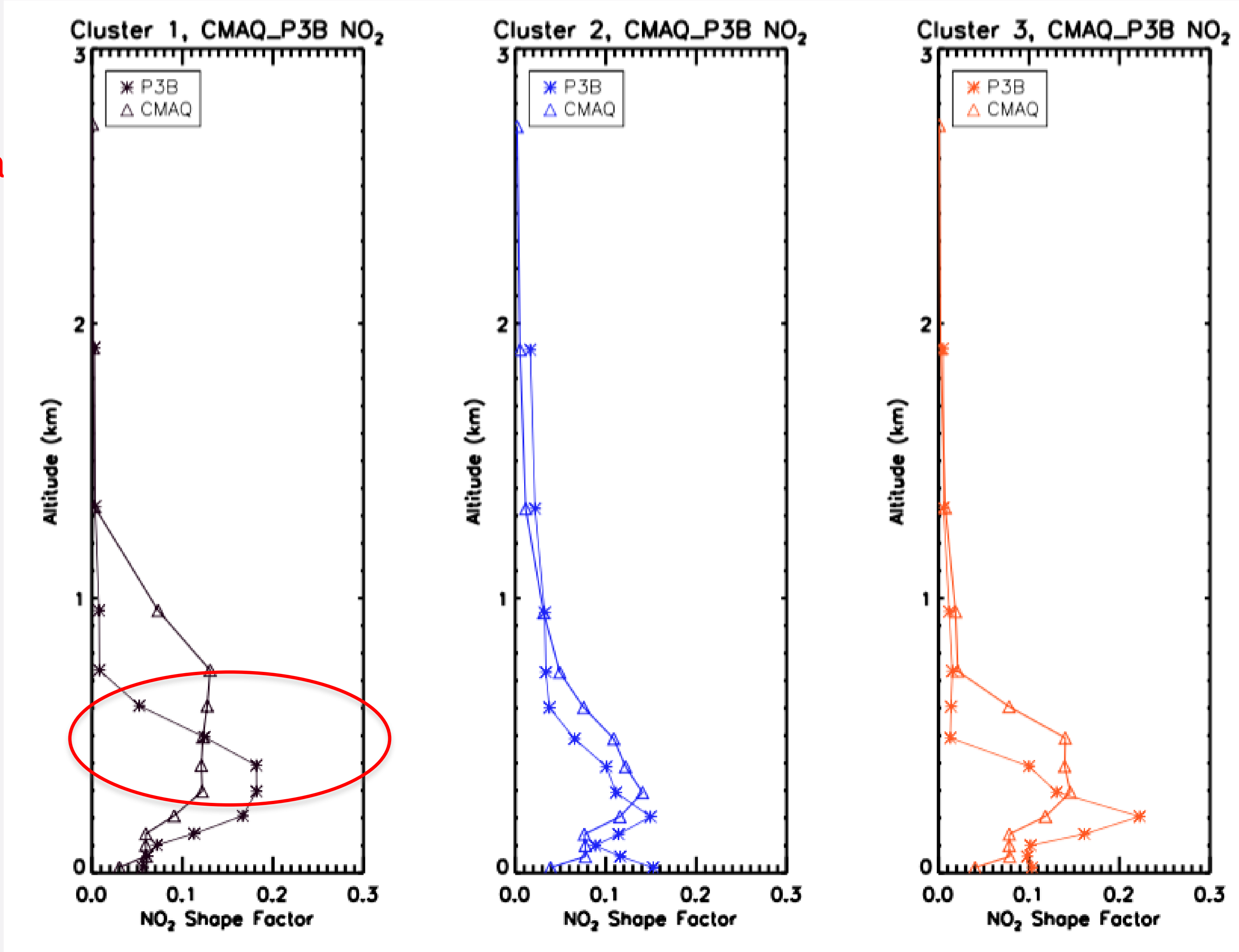
P3B/CMAQ O_3 Shape Factors

California



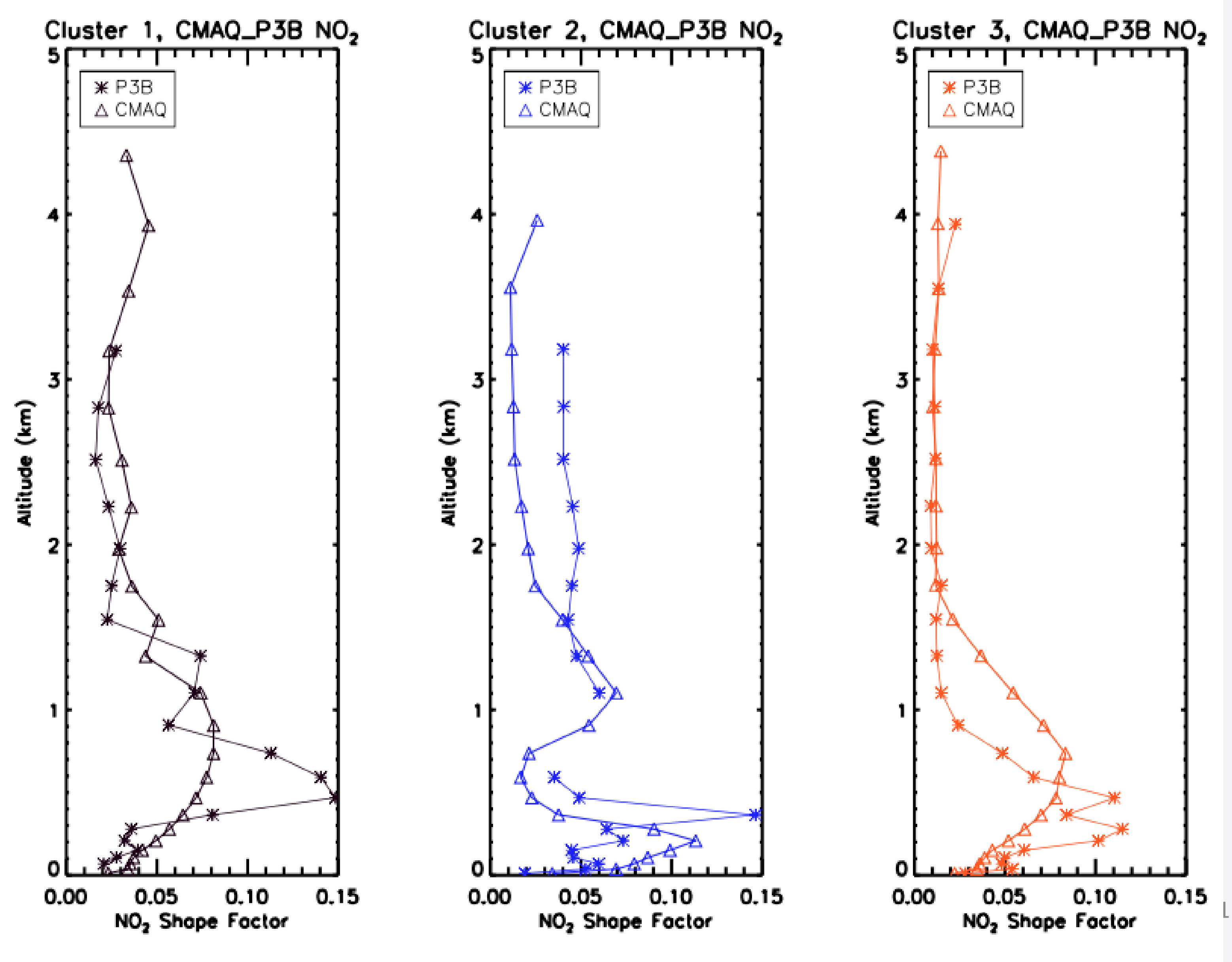
P3B/CMAQ NO_2 Shape Factors

California



P3B/CMAQ NO_2 Shape Factors

Texas



Conclusions

- P3B O_3 clusters:
  - Few terrain influences, and generally westerly flow at several layers leads to little variability of profile shapes -- Maryland
  - Cold season and/or terrain influences dampen variability, though not as much as for Maryland
  - Atmospheric stability influences median cluster profile shape

- P3B NO_2 clusters:
  - NO_2 displayed relatively uniform behavior for the MD, TX campaigns (due to O_3 production?) and CO campaign
  - California displayed the greatest amount of variability

Conclusions

- P-3B O_3 cluster shape factors:
  - CMAQ shape factors generally capture the shape and magnitude of the P-3B shape factors
- P-3B NO_2 cluster shape factors:
  - CMAQ captures some of the structure of the P-3B shape factors, though generally too smooth relative to P-3B within PBL
  - CMAQ shape factors thus too large or too small relative to observations, depending on altitude and cluster
- These shape factor profiles indicate that CMAQ remains too well mixed in the vertical
  - Shape factor error more critical in FT than PBL, where OMI-like instruments are more sensitive to composition
  - Indicates greater error for less well mixed gases such as NO_2